Journal of Molecular Structure (Theochem), 228 (1991) 353
Elsevier Science Publishers B.V., Amsterdam

AUTHOR INDEX

Abronin, I.A., 19
Aihara, J.-I., 277
Alcolea Palafox, M., 315
Alkorta, I., 47
Avdyuhina, N.A., 19

Badawi, H.M., 159
Balaban, A.T., 47
Balcioğlu, N., 323
Benassi, R., 71
Bochicchio, R.C., 209, 227
Boggs, J.E., 315
Boudon, S., 61

Cai, J., 181
Chandrasekhar, J., 249
Coussens, B., 335
Craw, J.S., 191

De Almeida, W.B., 191
De Gambiagi, M.S., 305
Decleva, P., 97

Elguero, J., 47

Firat, T., 323
Folli, U., 71
Fronzoni, G., 97

Geise, H.J., 27
Giambiagi, M., 305
Gu, J.-P., 87
Guo, Y., 285

Hagler, A.T., 237
Hinchliffe, A., 191
Honda, M., 201
Huang, M.-B., 87

Ishizuka, N., 259

Karpas, Z., 237
Khaikin, L.S., 315
Komiha, N., 11
Kong, F., 87
Kysel, O., 349

Ladik, J., 271
Leroy, G., 37
Lhamyani-Chraibi, M., 11
Lin, M., 139
Lisini, A., 97
Liu, S.-H., 87
Loar, G.W., 167

Mach, P., 349
Magomedov, G.K.-T., 19
Mestechkin, M., 117
Moc, J., 131
Morozova, L.V., 19
Mucci, A., 71

Ooms, K., 335
Otto, P., 271

Peeters, A., 27
Perevozchikov, V.I., 315
Pestunovich, V.A., 1
Pires, J.M., 305

Ratajczak, H., 131
Rathna, A., 249
Ríos, M.A., 149
Rodríguez, J., 149
Rozas, I., 47
Rudziński, J.M., 131

Sana, M., 37
Schenetti, L., 71
Sidorkin, V.F., 1
Siv'akova, L., 117
Sordo, J.A., 343
Sordo, T.L., 343
Stern, P.S., 237
Sussman, F., 237
Sutjianto, A., 271

Tachibana, A., 259
Taddei, F., 71
Tajima, M., 201
Topsom, R.D., 181
Tuan, D.F.-T., 167

Ünaleroğlu, C., 323

Van Alsenoy, C., 27
Vanquickenborne, L.G., 335
Vladimirov, V.V., 1
Voronkov, M.G.,

Whitehead, M.A., 285
Wilante, C., 37
Wipff, G., 61
Woolley, R.G., 329

Yamabe, T., 259

Zhang, Q., 139

Journal of Molecular Structure (Theochem), 228 (1991) 355–357
Elsevier Science Publishers B.V., Amsterdam

SUBJECT INDEX

Acetylene hydrogen-bonded tetramer
Ab initio study of the stationary points on the potential energy surface for the acetylene hydrogen-bonded tetramer, 191
Adenosine triphosphate
Molecular orbital study on the hydrolysis of adenosine triphosphate: the role of a cation as catalyst, 201
AlH_2
Ab initio study of some doublet excited states of AlH_2, 87
Aliphatic side chains
Improved band structures of some homopolypeptides with aliphatic side chains and of the four nucleotide base stacks: estimation of their fundamental gap, 271
Amino-acids
Hardness of amino-acids, 305
2-Aminoethenol 2-iminoethanal complex
Ab initio study of double proton transfer in the 2-aminoethenol 2-iminoethanal complex, 259
Aminosulphuric acid
Ab initio geometries and frequencies for aminosulphuric acid, $H_2NSO_2(OH)$, and the sulphamate anion, $H_2NSO_3^-$, 329
Annelated three-membered rings
An ab initio gradient study of the molecular geometry of some strained hydrocarbons containing annelated three-membered rings, 27

Carbene and its analogue complexes
MNDO calculations of carbene and is analogue complexes with chromium pentacarbonyl, 19
Cation as catalyst
Molecular orbital study on the hydrolysis of adenosine triphosphate: the role of a cation as catalyst, 201
Chromium pentacarbonyl
MNDO calculations of carbene and is analogue complexes with chromium pentacarbonyl, 19
Cis-trans isomerization
Cis-trans isomerization of protonated formaldehyde and its fluoro and chloro substituents, 237
CN^-
Theoretical studies of the photoionisation spectrum and the ultraviolet spectrum of the CN^- anion (in French), 11
Cyclopropylcarboxaldehyde
Conformational equilibria and structure of cyclopropylcarboxaldehyde and 1-methyl and 1-halo derivatives, 159

1,3,2-Dioxaphospholene
Conformational changes by ring puckering and inversion in 1,3,2-dioxaphospholene, 315
Dodecahedrane
Theoretical studies of aza analogues of platonic hydrocarbons. Part III. Dodecahedrane and its aza derivatives, 47
Doublet excited states
Ab initio study of some doublet excited states of AlH_2, 87
Double proton transfer
Ab initio study of double proton transfer in the 2-aminoethenol 2-iminoethanal complex, 259

Enthalpies of formation
The enthalpies of formation of substituted methyl radicals: a theoretical contribution, 37
Exocyclic C–C bond contraction
MNDO study of coupled strained hydrocarbons: additivity of exocyclic C–C bond contraction induced by different ring systems, 249

Formaldehyde
Cis-trans isomerization of protonated formaldehyde and its fluoro and chloro substituents, 237
Furan and thiophene rings
Conformational preference of the methylsulphinyl group bonded to the furan and thiophene rings: a theoretical approach, 71

1-Halo derivatives
Conformational equilibria and structure of cyclopropylcarboxaldehyde and 1-methyl and 1-halo derivatives, 159
Hartree–Fock–Roothaan SCF wavefunctions
On quality tests for Hartree–Fock–Roothaan SCF wavefunctions, 335
HFS constants
Effect of polar medium on the HFS constants of the $H_2NO^{\cdot}$ radical: ab initio continuum model study, 349
$H_2NO^{\cdot}$ radical
Effect of polar medium on the HFS constants of the $H_2NO^{\cdot}$ radical: ab initio continuum model study, 349
Homopolypeptides
Improved band structures of some homopolypeptides with aliphatic side chains and of the four nucleotide base stacks: estimation of their fundamental gap, 271

Interstellar molecules
Topological charge stabilization and interstellar molecules, 277
Intramolecular hydrogen bond
Analysis of the effect of substitution on the intramolecular hydrogen bond of malonaldehyde by ab initio calculations at the 3-21G level, 149

$[M_6X_8]n+$
Electronic structures of octahedral cluster halides of transition metals $[M_6X_8]^{n+}$, $[M_6X_{12}]^{n+}$ and their interstitial compounds $[M_6X_{12}Z]$, 139
$[M_6X_{12}]n+$
Electronic structures of octahedral cluster halides of transition metals $[M_6X_8]^{n+}$, $[M_6X_{12}]^{n+}$ and their interstitial compounds $[M_6X_{12}Z]$, 139
$[M_6X_{12}Z]$
Electronic structures of octahedral cluster halides of transition metals $[M_6X_8]^{n+}$, $[M_6X_{12}]^{n+}$ and their interstitial compounds $[M_6X_{12}Z]$, 139
Malonaldehyde
Analysis of the effect of substitution on the intramolecular hydrogen bond of malonaldehyde by ab initio calculations at the 3-12G level, 149

MC-SCF/CI model
Quantum statistical nature of the chemical bond. Part II. MC-SCF/CI model, 227
1-Methyl derivatives
Conformational equilibria and structure of cyclopropylcarboxaldehyde and 1-methyl and 1-halo derivatives, 159
Methylsulphinyl group
Conformational preference of the methylsulphinyl group bonded to the furan and thiophene rings: a theoretical approach, 71

NH_3
Corrections for overlapping spheres in the self-consistent field $X\alpha$ scattered wave method. Part 2. Application to NH_3, 167
Nucleotide base stacks
Improved band structures of some homopolypeptides with aliphatic side chains and of the four nucleotide base stacks: estimation of their fundamental gap, 271

Octhahedral cluster halides
Electronic structures of octahedral cluster halides of transition metals $[M_6X_8]^{n+}$, $[M_6X_{12}]^{n+}$ and their interstitial compounds $[M_6X_{12}Z]$, 139

Photoionisation spectrum
Theoretical studies of the photoionisation spectrum and the ultraviolet spectrum of the CN^- anion, 11
Platonic hydrocarbons
Theoretical studies of aza analogues of platonic hydrocabons. Part III. Dodecahedrane and its aza derivatives, 47
Polycyclic hydrocarbons
Activity indices of polycyclic hydrocarbons, 117
Population analysis
Quantum statistical nature of the chemical bond. Part I. Theoretical framework of population analysis and application to SCF closed shell wavefunctions, 209
Potential energy surface
Ab initio study of the stationary points on the potential energy surface for the acetylene hydrogen-bonded tetramer, 191
Protonated ethylendiamine

Conformational analysis of protonated ethylenediamine in the gas phase and in water, 61

δ quality test
Some comments on the δ quality test, 343

Ring puckering and inversion
Conformational changes by ring puckering and inversion in 1,3,2-dioxaphospholene, 315

SCF closed shell wavefunctions
Quantum statistical nature of the chemical bond. Part I. Theoretical framework of population analysis and application to SCF closed shell wavefunctions, 209

Second and third row hydrides
Theoretical study of the satellite structure in the valence photoelectron spectra of the second and third row hydrides, 97

Self-consistent field Xα scattered wave method
Corrections for overlapping spheres in the self-consistent field Xα scattered wave method. Part 2. Application to NH_3, 167

Self-interaction corrected multiple-scattering X_α method
Self-interaction corrected multiple-scattering X_α method: application to molecules, 285

SiH_5 species
Ab initio study of the SiH_5 species, 131

Silicon(IV) atom
Modelling of the pathway of S_N2 intramolecular substitution at the silicon(IV) atom, 1

Sliding-range method
A new approach to the geometry optimization of molecular structures: the sliding-range method, 323

S_N2 Intramolecular substitution
Modelling of the pathway of S_N2 intramolecular substitution at the silicon(IV) atom, 1

Strained hydrocarbons
An ab initio gradient study of the molecular geometry of some strained hydrocarbons containing annelated three-membered rings, 27

Substituent resonance effects
The influence of water on substituent resonance effects, 181

Substituted methyl radicals
The enthalpies of formation of substituted methyl radicals: a theoretical contribution, 37

Sulphamate anion
Ab initio geometries and frequencies for aminosulphuric acid, $H_2NSO_2(OH)$, and the sulphamate anion, $H_2NSO_3^-$, 329

Topological charge stabilization
Topological charge stabilization and interstellar molecules, 277

Ultraviolet spectrum
Theoretical studies of the photoionisation spectrum and the ultraviolet spectrum of the CN^- anion, 11

Valence photoelectron spectra
Theoretical study of the satellite structure in the valence photoelectron spectra of the second and third row hydrides, 97